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Infinite spherical well as model of quantum carnot engine

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Abstract

The potential well is a simple example that generally used to present an understanding of quantum mechanics. In this article, we used infinite spherical well model to evaluate the thermodynamic processes in a quantum Carnot engine. The energy of the particles depended on the value of n and l lead to complex calculations. For simplicity we used the φ_{100} and φ_{200} quantum states to determine work and efficiency of a quantum Carnot machine. The results obtained show that efficiency depends on the value of γ which is the ratio of R_C and R_B.

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INTRODUCTION

Classically a heat engine converts heat energy into mechanical work. The gas in the engine can expand and compress the system. One of these heat engines is the Carnot engine. The Carnot engine works through four thermodynamic cycles, specifically two isothermal cycles and two isobaric cycles. The efficiency η of the heat engine can be obtained using the equation

$$\eta = \frac{W}{Q_K}, \tag{1}$$

where W and Q_K are the work and heat absorbed by the heat engine respectively.

Since the beginning of the quantum era, physicists have tried to find a relationship between classical physics and quantum physics. One of them is the quantum characteristics of thermodynamic processes. Thermodynamic processes such as isobaric, isovolume, isothermal and adiabatic have been studied in (Bender et al., 2000), (Goswami & Harbola, 2013), (Quan et al., 2007), (Quan, 2009), (Papadatos & Anastopoulos, 2020), (Macchiavello et al., 2020) and (Çakmak & Müstecaplloğlu, 2019). One of the models used to explain the quantum nature of the thermodynamic process is the infinite well potential. The infinite potential well provides simplicity for obtaining solutions to the Schrodinger equation. Various cases have been studied using infinite potential well systems such as box potential well with movable walls (Koehn, 2012) and box potential well with oscillating wall

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(Glasser et al., 2009). Furthermore, the infinite potential well is also used as a model to describe the quantum heat engine system (Bender et al., 2000; Rezek & Kosloff, 2006; Thomas et al., 2019; Xu et al., 2018; Muñoz & Peña, 2012; Sutantyo, 2020; Sutantyo et al., 2015).

METHOD

In this article we use an infinite spherical well in evaluating the thermodynamic cycle, work and efficiency for quantum Carnot engine. Therefore, we evaluate some of the thermodynamic processes in the Carnot engine in several stages. This article structured as follows; first we describes the energy and wave function of an infinite spherical well, second we describes the quantum Carnot cycle which consists of two isothermal processes and two adiabatic processes and finally we discusses the work and efficiency of a quantum Carnot engine.

Energy And Wave Function

In this article we use an infinite spherical well as a model for determining the quantum Carnot cycle. The potential function of the infinite spherical well is

$$V(r) = \begin{cases} 0, & r < R, \\ \infty, & r > R. \end{cases} \tag{2}$$

In this model, the motion of the particles is restricted to the surface of the potential sphere so that the wave function vanishes outside the sphere. Using spherical coordinates in the Schrodinger equation, the radial equation for an infinite potential well is given by

$$\frac{d^2U(r)}{dr^2} = \left[\frac{l(l+1)}{r^2} - k^2\right]U(r), \tag{3}$$

where $k = \frac{\sqrt{2mE}}{\hbar}$ dan $U(r) = r\,R(r)$**.** Generally the solution to equation (2) is

$$U(r) = Pr\,J_l(kr) + Qr\,N_l(kr), \tag{4}$$

where $J_l(kr)$ and $N_l(kr)$ is called Bessel and Neumann function respectively. Function $J_l(kr)$ and $N_l(kr)$ are defined as

$$J_l(kr) = (-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\sin x}{x} \tag{5}$$

$$N_l(kr) = -(-x)^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{cos\,x}{x}. \tag{6}$$

The values of the constants P and Q can be obtained using boundary conditions. At this boundary condition the wave function will be zero. Note that when $r \to 0$, the Neumann function will be blow up. Hence the constant B must be zero. Thus equation (4) becomes

$$R(r) = Pr\,J_l(kr). \tag{7}$$

By using the boundary conditions $r = R$, equation (7) becomes

$$J_l(kr) = 0. \tag{8}$$

The conditions that satisfy equation (8) are

$$k = \frac{\rho_{nl}}{R}, \tag{9}$$

where ρ_{nl} is the n-th zero value of the l-th order Bessel function. The above equation gives the result

$$E_{nl} = \frac{\hbar^2}{2mR^2}\rho_{nl} \tag{10}$$

and eigen function

$$\varphi_{nlm} = A_{nl}\, J_l\left(\frac{\beta_{nl}\, r}{R}\right)\, Y_l^m(\theta, \phi), \tag{11}$$

where Y_l^m is spherical harmonic function. The wave function of particle can be expressed in a linear combination of equation (11) that is

$$\psi = \sum a_{nlm}\varphi_{nlm} \tag{12}$$

And coefficient *a_nlm* in equation (12) above satisfies the condition

$$|a_{100}|^2 + |a_{200}|^2 + \cdots + |a_{110}|^2 + \cdots = 1. \tag{13}$$

The expectation energy of particle given by

$$E = \sum |a_{nlm}|^2 E_{nl}. \tag{14}$$

For l = m = 0, energy and quantum state of the particle are

$$E_{n0} = \frac{n^2\pi^2\hbar^2}{2mR^2}, \tag{15}$$

$$\varphi_{n00} = \frac{1}{\sqrt{2\pi R\, r^2}} sin\left(\frac{n\pi}{R} r\right) \tag{16}$$

where normalized conditions have been used for the constant

$$A_{n0} = \sqrt{\frac{2}{R}}$$

and the spherical harmonic function

$$Y_0^0 = \sqrt{\frac{1}{4\pi}}.$$

In this article the discussion will be limited to the quantum state of the particle from the ground state φ_{100} and excited φ_{200}.

Quantum Carnot Cycle

The Carnot engine consists of four thermodynamic cycles, namely two isothermal cycles and two adiabatic cycles. In isothermal cycle, the system is always in thermal equilibrium. This can happen if during the process the particles remain in contact with the hot reservoir T_H. The first law of thermodynamics for isothermal processes is given by

$$dQ = dW. \tag{17}$$

In an adiabatic cycle, no heat enters or leaves the system. In this process the particles do not have to come into contact with the hot reservoir T_H. In an adiabatic process, the first law of thermodynamics is given by

$$-dU = dW. \tag{18}$$

The force generated in each process is given by

$$F = -\nabla E. \tag{19}$$

This article discusses systems in spherical coordinates and since the quantum energy depends only on distance, the above forces become

$$F = -\frac{dE}{dr}. \tag{20}$$

The following is a description of the four quantum Carnot cycles for the infinite potential spherical model.

Isothermal Process *A*-*B*

In this process, the system expands while in contact with the heat reservoir T_H so that the system temperature is in thermal equilibrium. During an isothermal process, the coefficient a_{nlm} is not constant and the system is excited. The quantum state of the system in this process given by

$$\psi = a_{100}\sqrt{\frac{1}{2\pi R r^2}}\sin\left(\frac{\pi r}{R}\right) + a_{200}\sqrt{\frac{1}{2\pi R r^2}}\sin\left(\frac{2\pi r}{R}\right). \tag{21}$$

The boundary condition for the coefficients in equation (13) is given by

$$|a_{100}|^2 + |a_{200}|^2 = 1. \tag{22}$$

Using equation (14) and boundary conditions (22), the expectation energy of the particle in an isothermal process can be expressed as

$$E = (4 - 3|a_{100}|^2)\frac{\pi^2\hbar^2}{2mR^2}. \tag{23}$$

The energy E in equation (23) is equal to the energy possessed by the particles throughout the isothermal process *A*-*B* (15) and gives a relationship between R and R_A, namely

$$R^2 = (4 - 3|a_{100}|^2)R_A^2. \tag{24}$$

Using equations (20) and (24), the force exerted during the isothermal process *A*-*B* is

$$F_{AB} = \frac{\pi^2\hbar^2}{mR_A^2 R}. \tag{25}$$

The maximum distance that can be carried by the force F_{AB} during isothermal process *A*-*B* is when

$$R = R_B = 2R_A.$$

When the particle is in R_B, the coefficient a_{100} = 0 and indicates that the particle is in a pure excited state. Furthermore at the maximum distance, the quantum state of the particle becomes

$$\psi = \sqrt{\frac{1}{2\pi r R_B^2}} \sin\left(\frac{2\pi r}{R_B}\right) \tag{26}$$

and energy of particle is

$$E_{20} = \frac{4\pi^2\hbar^2}{2mR_B^2}. \tag{27}$$

Adiabatic Process *B-C*

During an adiabatic process there is no heat change in the system. There is no energy received or dissipated by the system. The quantum state and the coefficient a_{200} of the system in this process remain constant. Furthermore the quantum state of the particle in this process is given by

$$\psi = \sqrt{\frac{1}{2\pi a R_B^2}} sin\left(\frac{2\pi r}{R_B}\right) = \sqrt{\frac{1}{2\pi a R_C^2}} sin\left(\frac{2\pi r}{R_C}\right), \tag{28}$$

and energy of the particle along the adiabatic process *B-C* is

$$E_{20} = \frac{4\pi^2\hbar^2}{2mR^2}. \tag{29}$$

the force exerted during this process is

$$F_{BC} = \frac{4\pi^2\hbar^2}{mR^3}. \tag{30}$$

Assume that the ratio between R_C and R_B is equal to γ, then the energy at R_C is given by

$$E'_{20} = \frac{4\pi^2\hbar^2}{2mR_C^2} = \frac{E_{20}}{\gamma^2}. \tag{31}$$

Isothermal Process *C-D*

In the isothermal process *C-D* the system is compressed while in contact with the heat reservoir T_H so that the system is in thermal equilibrium. The quantum state of the system and the coefficients a_{nlm} are not constant during this process. We choose the final state of the particle in this process back to the elementary quantum state. Furthermore the wave function and the expectation energy of the particle are respectively given by

$$\psi = a_{100}\sqrt{\frac{1}{2\pi R r^2}} \sin\left(\frac{\pi r}{R}\right) + a_{200}\sqrt{\frac{1}{2\pi R r^2}} \sin\left(\frac{2\pi r}{R}\right), \tag{32}$$

$$E = (4 - 3|a_{100}|^2)\frac{\pi^2\hbar^2}{2mR^2}. \tag{33}$$

Using equations (29) and (33) the relationship between R_C and R during isothermal processes *C-D* is given by

$$R^2 = \frac{4 - 3|a_{100}|^2}{4} R_C^2. \tag{34}$$

The force exerted during this process is

$$F_{CD} = \frac{4\pi^2\hbar^2}{mR_C^2 R}. \tag{35}$$

During isothermal process *C-D*, the maximum distance that can be obtained when

$$R = R_D = \frac{R_C}{2}. \tag{36}$$

At this point the particle is completely excited, so the quantum state and the expectation energy of particle become

$$\psi = \sqrt{\frac{1}{2\pi R_D^2}} \sin\left(\frac{\pi r}{R_D}\right) \tag{37}$$

$$E_{10} = \frac{\pi^2\hbar^2}{2mR_D^2}. \tag{38}$$

Adiabatic Process *D-A*

In this process the system will be compressed until the particle returns to R_A. The quantum state and the constant a_{nlm} of this process remain constant. Furthermore the energy possessed by the particles during the adiabatic process *D-A* is the same as equation (38). The force required throughout this process is

$$F_{DA} = \frac{\pi^2\hbar^2}{mR^3}. \tag{39}$$

Work And Efficiency Of The Quantum Carnot Engine

The total work produced during the four Carnot cycles is given by

$$\mathrm{W} = \int_{\mathrm{R_A}}^{\mathrm{R_B}} \mathrm{F_{AB}}\, \mathrm{dR} + \int_{\mathrm{R_B}}^{\mathrm{R_C}} \mathrm{F_{BC}}\, \mathrm{dR} + \int_{\mathrm{R_C}}^{\mathrm{R_D}} \mathrm{F_{CD}}\, \mathrm{dR} + \int_{\mathrm{R_D}}^{\mathrm{R_A}} \mathrm{F_{DA}}\, \mathrm{dR}$$

$$W = \frac{\pi^2\hbar^2}{mR_A^2} \ln 2\left(1 - \frac{1}{\gamma^2}\right) \tag{40}$$

To determine the efficiency of a Carnot engine, it is necessary to find the amount of heat absorbed by the system while the particle is undergoing a quantum Carnot cycle. The heat absorbed by the system occurs in isothermal processes *A-B*. Furthermore the amount of heat absorbed given by

$$Q_K = \int_{R_A}^{R_B} F_{AB}(R)\, dR$$

$$Q_K = \frac{\pi^2\hbar^2}{mR_A^2} \ln 2. \tag{41}$$

Using equations (40) and (41) the efficiency of the quantum Carnot engine of this system is

$$\eta = 1 - \frac{1}{\gamma^2}, \tag{42}$$

where γ is the ratio of R_C and R_B. Equation (42) gives different results to the classical Carnot engine, where efficiency can depend on hot and cold reservoir temperatures.

RESULTS AND DISCUSSION

Equation (42) shows that the efficiency of a quantum Carnot engine using the infinite ball well model only depends on the size of the potential ball well due to isothermal expansion R_C and adiabatic expansion R_B. This is different from the classic Carnot engine which depends on the temperature of the hot and cold reservoirs of the engine. In obtaining equation (42), we constrain that the quantum state of the particle during the isothermal process *C-D* returns to the initial quantum state. Even though the quantum state of the particle returns to its initial state, the energy of the particle has a different value, namely equations (27) and (38).

Using the quantum states φ_{100} and φ_{200} in our model, we find that the efficiency of the quantum Carnot engine has the same shape as the one-dimensional potential well model. This result occurs because we only take the boundary condition where the value $l = m = 0$. This condition reduces the Bessel and Newman function in equation (4) to a one-dimensional potential well wave equation. Thus the particle energy only depends on the value of n.

CONCLUSION

We have evaluated the thermodynamic cycle for the quantum Carnot engine using the infinite spherical potential model. Moreover, the work and efficiency of the quantum Carnot engine are also evaluated. In contrast to the common models such as one-dimensional and three-dimensional infinite box potentials, the energy of the particles inside an infinite spherical well depended on the values of n and l as shown in equation (10). In addition, the quantum state of the particles also have distinction. For simplify, we found that the work and efficiency of the Carnot quantum machine remains the same as the one-dimensional box potential. The discussion become more complicated by calculating the possibilities for the l and m values of the quantum state obtained by the infinite potential spherical model.

Further research can be conducted using this model by extending again and taking the value $l = m \neq 0$. Using the condition, the quantum state of the particles becomes a superposition of various values of n, l and m are used and the energy of the particles depends on the values of n and l.

AUTHOR CONTRIBUTIONS

Conceptualization, investigation and writing-original manuscrip preparation, K Fahmi; formal analysis, K Fahmi, A.T Oktaviana.

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